Dynamical Solutions to the Ground State of a Frustrated Magnet*

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Abstract: This project explores a computational approach to simulating a frustrated antiferromagnetic system, using a simplified Ising model on a triangular lattice.[1, 2] By exhaustively scanning all possible spin configurations, we identified the ground states of the system and uncovered the local constraints that give rise to frustration.[3, 4] Building on these results, we developed a technique to extract spin-spin correlations directly from the amplitudes of the ground state basis, allowing us to probe how individual dipoles interact across the lattice.[5, 6] This analysis revealed which spins are most entangled in the system's frustration and how local behavior shapes the global magnetic structure.[5] These findings lay the groundwork for more advanced quantum simulations and can inform future research into the behavior of frustrated magnetic systems.[3, 7]

I - Introduction

Frustrated magnet systems have garnered significant interest due to the complex and unique phenomena they exhibit.[3, 4, 8] These systems pose considerable challenges for classical simulation methods, particularly in approximating and identifying their true ground states.[3, 9] The difficulty arises from the vast number of spin configurations with nearly degenerate energies, making it difficult to pinpoint the actual minimum-energy state.[3]

Magnetic frustration occurs when a system's spin interactions cannot all be simultaneously satisfied, often due to either geometric or energetic constraints.[3, 4, 10] This leads to a highly degenerate set of low-energy states and prevents the system from settling into a simple, ordered configuration. A classic example is the antiferromagnet on a triangular lattice.[1, 2, 10] In such a system, each spin seeks to align opposite to its neighbors, but due to the triangular geometry, it is impossible for all three spins in a triangle to align in opposite directions all at once. As a result, at least one bond in every triangle on the lattice must remain "unsatisfied", thus giving rise to frustration.[3]

From a computational perspective, simulating these systems is notoriously difficult.[3, 5, 9] The number of possible spin configurations grows exponentially with system size, and the presence of frustration makes the energy landscape rugged and densely populated with local minima. Traditional minimization techniques and Monte Carlo sampling often become inefficient or unreliable in these settings.[5, 9, 11]

To address this challenge, we explore a simplified model of frustration using an antiferromagnetic Ising model on a triangular lattice.[1, 2] By isolating the geometric source of frustration and using a tractable lattice structure, we aim to gain insight into the underlying physics of these systems without the added complexity of long-range interactions or external fields. Our approach involves calculating the exact ground states of small systems and analyzing spin-spin correlations to identify which dipoles are most affected by frustration. These results can serve as a foundation for more advanced simulations and may eventually guide the development of hybrid classical-quantum algorithms tailored for frustrated systems.[7]

Frustrated magnetic systems are not just theoretically interesting — they are closely related to exotic phases of matter such as spin

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glasses, spin liquids, and certain classes of high-temperature superconductors.[3, 8, 12, 13] These phases are characterized by nontrivial correlations, long-range entanglement, and emergent behaviors that defy conventional magnetic order.[12, 14] Although this project does not directly model these complex phases, understanding frustration at a fundamental level is a necessary step toward exploring such phenomena, both experimentally and computationally.

II - Background

Triangular lattices are a common testbed for studying frustration because their geometry naturally introduces competing interactions under antiferromagnetic coupling.[3, 4, 6] In contrast to square lattices — where all nearest-neighbor bonds can be satisfied — triangular units inherently prevent full anti-alignment, making them a minimal yet nontrivial frustrated system.[5] This behavior is illustrated in Figure 1.

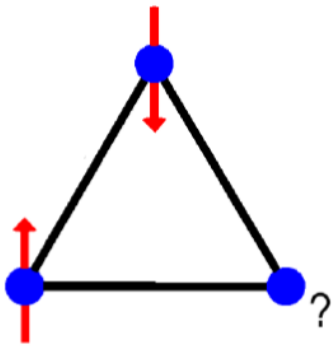

Figure 1: Frustrated spin configuration on a triangular lattice.[15]

This geometric frustration forms the basis of the system studied in this project. By arranging dipoles (spins) on a triangular lattice and enforcing antiferromagnetic coupling, we create a situation in which the system cannot simultaneously satisfy all local spin interactions. This gives rise to a highly degenerate set of low-energy states and a nontrivial magnetic landscape that is well-suited for computational investigation.[3, 4]

To model these interactions quantitatively, we adopt a simplified form of the Ising Hamiltonian, which allows us to compute the total energy of a given spin configuration based on local pairwise interactions.[2, 11] This formulation enables us to identify the minimum-energy state of the spin system as a whole:

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

In this Hamiltonian, $H(\sigma)$ represents the total energy of the system, J is the coupling constant, and σ_i and σ_j are the spin states of the individual dipoles. Each spin is represented by $+1$ (spin up) or -1 (spin down), and the total energy is calculated by summing over all pairwise spin interactions across the lattice.[11]

When analyzing a full system, each pair of neighboring spins contributes to the total energy based on their alignment. Parallel spins — either up-up ($+1 \times +1 = +1$) or down-down ($-1 \times -1 = +1$) — contribute positively to the interaction sum. In contrast, antiparallel spins (e.g., $+1 \times -1 = -1$) contribute negatively. The sign and magnitude of J determine how these contributions influence the system's total energy.[3]

While the magnitude of J can be chosen to scale the system appropriately, its polarity is particularly significant. If $J > 0$, the system energetically favors aligned spins, resulting in a ground state that is fully *ferromagnetic*. Conversely, if $J < 0$, the system favors antiparallel spins, yielding a ground state that is fully *antiferromagnetic*.[3] This distinction is crucial when modeling frustration, as the preferred spin alignment can directly conflict with the geometry of the lattice. For the purposes of this project — simulating a frustrated antiferromagnetic system — we used $J = -1$.

Although the simplified Ising model captures the essential interactions driving frustration, more complete versions of the model in-

corporate additional physical effects — such as external magnetic fields or long-range interactions — that can significantly alter the system's behavior and ground state structure.[3, 5] The full form of the Ising model typically includes an external magnetic field term, anisotropic couplings, or interactions beyond nearest neighbors:

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{2}$$

where h is the strength of the external magnetic field, and the notation $\langle i, j \rangle$ indicates that the sum is taken over nearest-neighbor pairs. The simplified version omits these complexities, focusing exclusively on uniform nearest-neighbor interactions without external fields or anisotropies.[11]

This simplification is beneficial for several reasons. First, it allows us to isolate and study the effects of geometric frustration without additional influences from external fields. Second, it enables exhaustive exploration of the system's configurations, as the energy landscape becomes more tractable for small lattice sizes.[5, 11] Finally, the simplified model serves as a useful baseline from which more complex interactions can be introduced incrementally in future simulations if desired.

In the context of frustrated systems, this model is particularly well-suited because the frustration arises from the geometry of the lattice itself — in this case, a triangular lattice — rather than from competing field interactions.[3, 4] By focusing on the intrinsic frustration due to lattice connectivity, the simplified Ising model provides a clear and computationally efficient means of investigating the emergent behavior of such systems.

Another significant component of this project involved quantifying correlations between specific dipoles to better understand the system's magnetic structure. This is particularly important because, once we determine how strongly one spin is correlated with another, we can more easily identify which dipoles are most frustrated within the lattice.[5, 6] To compute these correlations, we use Pauli's spin operators — specifically the σ_z operator: [16]

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Defining the system's quantum state as $|\psi\rangle$, we can calculate the spin-spin correlation function in the z-direction between dipoles "i" and "j" using the two-point expectation value: [17]

$$C_{ij} = \langle\, \psi \mid \sigma_z^{(i)} \otimes \sigma_z^{(j)} \mid \psi \,\rangle \tag{3}$$

This quantum spin-spin correlation function provides insight into the degree of alignment between different dipoles. A value of $C_{ij} \approx 1$ indicates that the spins are strongly aligned (i.e., correlated) with one another, meaning both are either in the up direction or the down direction. Conversely, a value of $C_{ij} \approx -1$ indicates that the spins are strongly anti-aligned, meaning their spins point in opposite directions. Values near zero suggest weak or no correlation, which may signal frustration within the system.[5]

For systems with more than two dipoles — such as the triangular lattice explored in this project — the spin-spin correlation function must account for all sites in the system. This is done by constructing a tensor product over all n dipoles, and inserting identity operators at positions not involved in the measurement.[17] Specifically, to compute the correlation between spins at sites "i" and "j", we define:

$$C_{ij} = \langle \psi | \sigma_z^{(i)} \otimes \sigma_z^{(j)} \otimes I^{(k)} \otimes \cdots \otimes I^{(n)} | \psi \rangle \tag{4}$$

Here, $\sigma_z^{(i)}$ and $\sigma_z^{(j)}$ act on sites "i" and "j", while $I^{(k)}$ through $I^{(n)}$ denote identity operators acting on all other dipoles in the system. The

full tensor product spans all n sites. This construction ensures that only the spins at sites "i" and "j" are acted upon by σ_z, while the remaining sites are left unchanged via the identity operator I. The result is a full-system operator that correctly evaluates the correlation between the two target dipoles in the context of the full quantum state $|\psi\rangle$.[17]

The simplified Ising model and quantum spin-spin correlations together form the theoretical foundation for the simulation methods described in the following section.

III - Methods

To investigate the ground state properties of a frustrated antiferromagnetic system, we developed a numerical simulation in Python using the NumPy library. The goal was to exhaustively explore all possible spin configurations of a small triangular lattice and identify those with the lowest total energy.[11]

To construct a triangular lattice, we began with a conventional $N \times M$ square lattice and imposed specific nearest-neighbor interaction rules. In particular, we added diagonal couplings between select neighbor pairs to emulate the triangular geometry.[3] Although this structure originates from a rectangular grid, the altered connectivity allows it to mirror the frustration-inducing features of a true triangular lattice. This choice offers an ideal balance between physical realism and implementation simplicity, since it avoids the need for irregular indexing schemes while still producing the desired geometric constraints.

In our implementation, each dipole interacts with the site immediately to its right, diagonally to the lower right, and directly below. These directional couplings ensure that every elementary unit of the lattice contains three spins forming a triangle, which is the minimum configuration required to introduce frustration under antiferromagnetic coupling.[5] When applied uniformly across the lattice, these interactions generate a repeating pattern of equilateral triangles, effectively simulating a triangular lattice, as illustrated in Figure 2. This structure serves as the foundation for all subsequent calculations of configuration energy and spin-spin correlations.

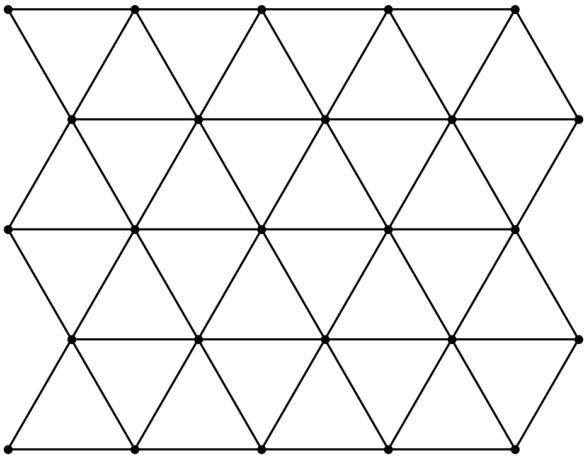

Figure 2: Triangular lattice generated from a square grid with directional interactions.

To better emulate an infinite lattice and minimize edge effects, periodic boundary conditions were applied to the system. This means that spins on the edges of the lattice interact with those on the opposite edge, effectively wrapping the lattice around both horizontally and vertically. In practice, this was implemented by applying modular indexing to each spin's neighbors when computing interaction energies. This wrapping ensures that every spin has the same number of neighbors, maintaining translational symmetry throughout the lattice.[11]

With a method to compute the energy of any given configuration established using the simplified Ising model, the next step was to generate all possible spin configurations in order to identify those corresponding to the ground state.[2, 11] To accomplish this, we implemented a function that converts bit strings into spin states, where "0" corresponds to spin up ($+1$) and "1" to spin down (-1).

For example, consider a rectangular lattice with dimensions $N = 3$ and $M = 5$. The total number of configurations is $2^{N\times M} = 2^{15} = 32{,}768$. Configuration 0 is represented in binary as `00000 00000 00000`, configuration 1 as `00000 00000 00001`, configuration 2 as `00000 00000 00010`, and so on, up to configuration 32,767 as `11111 11111 11111`.

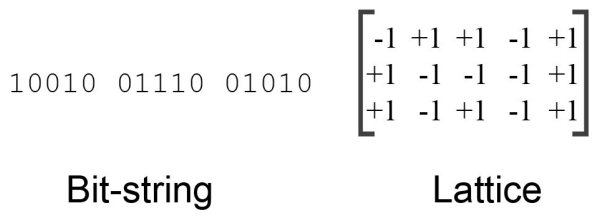

Figure 3: Mapping a binary bit string to a spin configuration on a 3×5 lattice.

Each configuration is represented as a bit string ordered in row-major fashion (left to right, top to bottom), where each bit corresponds to a site on the lattice. This bit-string representation is compact, easily indexable, and directly maps to binary integers, allowing for efficient iteration.

This representation allowed us to iterate through all possible configurations efficiently for a given $N \times M$ grid and store any desired configurations for further analysis in the form of a bit string. Each bit string could then be converted into a NumPy array of spin values (± 1), and the total energy was computed using the simplified Ising Hamiltonian.[11]

The simulation evaluated the energy of every configuration and recorded those with the lowest total energy. While this brute-force method is computationally intensive and scales poorly with system size, it remains tractable for small lattices and guarantees exact identification of the ground state manifold.[5] This is significant, as the true ground state of the system is a quantum superposition of all configurations with minimum energy.[6]

With a method for obtaining the full ground state superposition established, the next step was to apply the spin-spin correlation function defined in Equations (3) and (4) of the Background section. However, initial attempts to implement this calculation using explicit tensor products quickly ran into computational difficulties.

Although most of the tensor components in these expressions are identity operators, the exponential scaling of the full tensor product still results in a prohibitively large matrix.[17] For example, consider a 3×3 lattice with $n = 9$ dipoles. The resulting operator from the tensor product has dimensions $2^n \times 2^n = 512 \times 512$. For a 4×4 lattice, the size explodes to $2^{16} \times 2^{16} = 65{,}536 \times 65{,}536$.

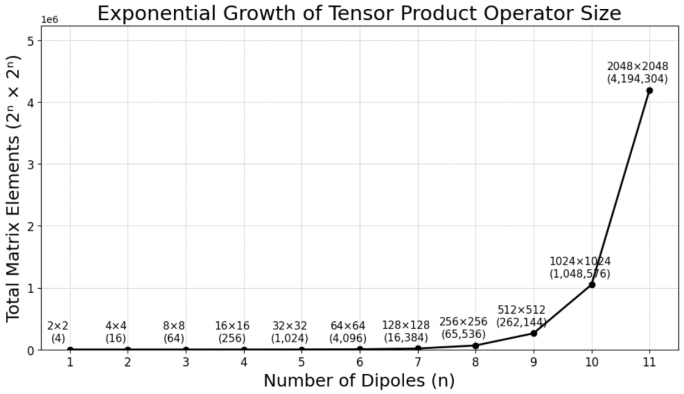

Figure 4: Growth of tensor product matrix size with number of dipoles. Matrix dimensions scale as $2^n \times 2^n$, growing exponentially with system size.

These dimensions do not even account for the construction of the quantum state vector $|\psi\rangle$, which in the 4×4 case is a $65{,}536 \times 1$ column vector. Moreover, generating this state vector involves performing a total of 16 successive tensor products — one for each spin in the lattice — further compounding the computational cost.

Taken together, this approach becomes extremely expensive and difficult to scale beyond roughly 9 dipoles. As a result, we

needed to develop an alternative method that is mathematically equivalent to the full tensor product formalism but avoids its computational pitfalls.

To address these computational limitations, we returned to the theoretical framework outlined in the Background section. In particular, we reconsidered how to represent the quantum state of the system in a form that avoids explicit tensor products.[16]

Rather than constructing the full state vector through successive Kronecker products, we instead defined the quantum state as a weighted sum over basis states corresponding to spin configurations. Each basis state represents a specific arrangement of up and down spins across the lattice, and the associated coefficient reflects its amplitude in the superposition. This formulation is shown in Equation (5): [17]

$$|\psi\rangle = \sum_{i,j\in\{0,1\}} \alpha_{ij}\,|ij\rangle \tag{5}$$

Here, $|ij\rangle$ denotes a basis state of the system, and α_{ij} is the complex amplitude associated with that configuration. This expression generalizes to n dipoles by summing over all 2^n basis states. The magnitude squared of each coefficient, $|\alpha_{ijk\cdots n}|^2$, gives the probability of measuring the system in the corresponding basis state $|ijk\cdots n\rangle$.

In the context of this project, we restrict our attention to the degenerate ground states of the system. Each of these ground-state configurations is assigned an equal amplitude, resulting in a normalized quantum state that is a uniform superposition over all lowest-energy spin arrangements. The normalization factor is $1/\sqrt{d}$, where d is the number of degenerate ground states.

To evaluate the spin-spin correlation function without explicitly constructing tensor product operators, we apply the definition of $|\psi\rangle$ from Equation (5) directly to the expectation value in Equation (3): [17]

$$C_{ij} = \langle\psi|\sigma_z^{(i)} \otimes \sigma_z^{(j)}|\psi\rangle \tag{6}$$

After a lengthy derivation — involving the expansion of the full quantum state in the computational basis, simplification of operator actions, and the use of the orthonormality of basis states (i.e., the Dirac delta property) — the correlation function reduces to a weighted sum over basis configurations. Each term in the sum reflects the probability of a given configuration and the product of the spin values at sites "i" and "j" within that configuration.[16] The final result is:

$$C_{ij} = \sum_{i,j\in\{0,1\}} |\alpha_{ij}|^2(-1)^i(-1)^j \tag{7}$$

Here, α_{ij} denotes the amplitude of the basis state $|ij\rangle$, and the factors $(-1)^i$ and $(-1)^j$ arise from the eigenvalues of the σ_z operator acting on qubits labeled by i and j. The eigenvalue of σ_z is $+1$ for spin-up (bit value 0) and -1 for spin-down (bit value 1), resulting in the $(-1)^b$ mapping from bit value to spin orientation.

While the expression above uses a 2-qubit example for clarity, the same reasoning extends naturally to systems with n dipoles. In that case, we sum over all 2^n basis states, each representing a complete spin configuration across the entire lattice. The correlation function is then computed by extracting the spins at sites "i" and "j" from each configuration, multiplying them, and weighting the result by the probability of that configuration in the quantum superposition.

This reformulated approach is particularly powerful because it entirely avoids the exponential overhead of building full tensor product operators. In the original formulation, constructing a two-point correlation function required building a $2^n \times 2^n$ matrix with σ_z acting

on sites "i" and "j", and identity operators elsewhere. In contrast, the basis-state formulation bypasses these identity components: since each basis state already encodes the full spin configuration, the effect of $\sigma_z^{(i)} \otimes \sigma_z^{(j)}$ is simply to contribute the classical product $\sigma_i \sigma_j$ for that configuration.[6]

Consequently, this method reduces the computation from matrix algebra over exponentially large operators to basic array processing: lookups, multiplications, and averages over a finite set of known configurations. It is significantly more efficient, scales well to larger system sizes, and retains exact correctness for any spin system modeled as a uniform superposition over classical ground states. As such, this reformulation is a central innovation of the project, allowing us to compute spin correlations efficiently and exactly without constructing large tensor product operators.

With this framework in place, we were able to analyze the structure of the ground state manifold and uncover how geometric frustration shapes the spin correlations across the lattice.

IV - Results

The simulation successfully identified the complete set of ground-state configurations for small frustrated antiferromagnetic lattices, and the spin-spin correlation analysis provided valuable insight into the internal structure of these states.[5] By reformulating the quantum state as a weighted superposition over ground-state basis vectors, we were able to compute pairwise spin correlations without resorting to full tensor product constructions.[16, 17] This approach significantly reduced computational overhead and enabled the analysis of systems with up to 16 dipoles — a meaningful step beyond what would be practical using conventional operator-based methods.[17]

The results illustrate a hallmark of magnetic frustration: while some dipole pairs exhibit strong correlations, others remain only weakly correlated or entirely uncorrelated.[3, 8] This variation reveals the presence of local frustration and highlights how geometric constraints prevent the system from settling into a globally ordered configuration.[4] Even in relatively small systems, we observe that spin alignment patterns are highly nonuniform, reflecting the underlying tension between interaction rules and lattice geometry. The correlation function served as a reliable and efficient tool for identifying which dipoles are most affected by this frustration.[5, 6]

A key outcome of this project is the demonstration that it is both possible and efficient to compute quantum observables — like the two-point correlation function — by working directly with basis states and their associated amplitudes.[17] This technique preserves the predictive power of the quantum formalism while avoiding the bottlenecks of explicit tensor algebra. By leveraging the structure of the ground-state manifold, the simulation remains accurate and scalable within the limits of classical computation.[9]

While the brute-force approach was sufficient for the small lattice sizes examined in this project, its exponential scaling limits its applicability to larger systems.[11] A natural next step would be to explore whether additional structure — such as symmetry or local conservation rules — could be used to reduce redundancy in the configuration space or classify distinct families of ground states.[5] These extensions would build on the framework developed here while extending its reach to more complex systems.

Due to time constraints, I was not able to fully explore the next phase of the project — namely, using the correlation results as a springboard for deeper physical analysis. In future work, I would aim to study how different patterns of spin-spin correlations emerge under varying lattice sizes, boundary conditions, or interaction rules. Additionally, finding effective ways to visualize this data

— such as heatmaps of C_{ij} values or spatial overlays on the lattice geometry — would allow for more intuitive interpretation of frustration and symmetry. These tools could help reveal whether emergent patterns exhibit any form of regularity, hidden symmetry, or sensitivity to local perturbations.[12]

Although I only completed debugging and validating each component of the simulation near the end of the project timeline, the core framework is now fully operational and provides a solid foundation for future investigation. With this infrastructure in place, the methods developed here can be extended toward broader studies of frustration, correlations, and emergent behavior in more complex magnetic systems.[8, 18]

V - Conclusion

This study demonstrated that a simplified Ising model on a triangular lattice effectively captures the essential features of geometric frustration in antiferromagnetic systems.[3, 4] By exhaustively enumerating spin configurations and calculating spin-spin correlations, we identified the degenerate ground states of small frustrated lattices and quantitatively assessed the patterns of frustration arising from incompatible local interactions.[5] Reformulating the quantum state as a superposition over classical basis states enabled the efficient computation of two-point correlation functions — without the need for exponentially large tensor products — thus extending the simulation's scalability to systems with up to 16 dipoles.[16, 17]

These results underscore two central insights: (1) geometric frustration leads to weak or fluctuating correlations between specific dipoles, even when all couplings are uniform and antiferromagnetic;[8] and (2) basis-state formulations offer a scalable and exact alternative to conventional tensor product methods for computing quantum observables.[6] The resulting correlation maps provide a clear framework for identifying regions of high frustration — so-called "hotspots" — which influence the magnetic structure of the system.

While the brute-force enumeration used in this study is effective for small lattices, its exponential scaling limits its applicability to larger systems.[11] Future work could explore more efficient strategies, such as symmetry-based sampling, energy-aware pruning of configuration space, or machine learning techniques to approximate ground-state distributions.[19] Additionally, extending the model to include quantum fluctuations (e.g., transverse fields) or anisotropic couplings, as provided by the full (non-simplified) Ising model, would offer a more complete picture of real-world frustrated materials.[12]

The computational framework developed here lays a solid foundation for future research into how frustration scales with system size and geometry — key questions for understanding emergent phases such as spin liquids.[8, 14] This work may also inform the development of quantum algorithms, guide experimental investigations of frustrated materials, or contribute to the design of systems where frustration is harnessed as a functional property.[7]

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